

Comparative Study of BCS-BEC Crossover Theories above T_c : the Nature of the Pseudogap in Ultra-Cold Atomic Fermi Gases

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This paper presents a comparison of two finite-temperature BCS-Bose Einstein condensation (BEC) crossover theories above the transition temperature: Nozieres Schmitt-Rink (NSR) theory and finite T -extended BCS-Leggett theory. The comparison is cast in the form of numerical studies of the behavior of the fermionic spectral function both theoretically and as constrained by (primarily) radio frequency (RF) experiments. Both theories include pair fluctuations and exhibit pseudogap effects, although the nature of this pseudogap is very different. The pseudogap in finite T -extended BCS-Leggett theory is found to follow a BCS-like dispersion which, in turn, is associated with a broadened BCS-like self energy, rather more similar to what is observed in high temperature superconductors (albeit, for a d -wave case). The fermionic quasi-particle dispersion is different in NSR theory and the damping is considerably larger. We argue that the two theories are appropriate in different temperature regimes with the BCS-Leggett approach more suitable nearer to condensation. There should, in effect, be little difference at higher T as the pseudogap becomes weaker and where the simplifying approximations used in the BCS-Leggett approach break down. On the basis of momentum-integrated radio frequency studies of unpolarized gases, it would be difficult to distinguish which theory is the better. A full comparison for polarized gases is not possible since there is claimed to be inconsistencies in the NSR approach (not found in the BCS-Leggett scheme). Future experiments along the lines of momentum resolved experiments look to be very promising in distinguishing the two theories.

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I. INTRODUCTION

The behavior of ultracold superfluid Fermi gases continues to attract attention from the experimental and theoretical communities. Through a Feshbach resonance [1, 2] which tunes the strength of the attractive interaction, these trapped gases can exhibit a crossover from BCS to Bose Einstein condensation (BEC). Unlike the Bose superfluids, at the time of their discovery, the Fermi superfluids are not associated with any ready-made theory (such as Gross Pitaevskii, or Bogoliubov theory for bosons). This provides an opportunity for theorists to work hand in hand with experimentalists to arrive at the same level of understanding of the fermionic as was reached for the bosonic superfluids. While the Fermi systems are harder to address than the Bose counterparts, the payoff for progress is great. Moreover, there is a general belief that these systems may lead to important insights into high temperature superconductor (HTSCs), in part because the HTSCs exhibit an anomalously short coherence length which suggests that they may be mid-way between BCS and BEC [3, 4, 5, 6].

There is, as yet, no clear consensus about the theory which underlies BCS-BEC crossover although there are three rather well studied analytic many body theories which have emerged. The goal of the present paper is to present a comparison and assessment of these approaches with a particular focus on the two of the three, which seem most reliable. In addition to assessing the theoretical approaches, we address physical consequences and how the theories may be differentiated through the behavior of the centrally important spectral function and related density of states. We do this in the context of radio-frequency-(RF) based probes.

What is among the most interesting features of BCS-BEC

crossover is the fact that the normal state (out of which superfluidity forms) is different from the normal state (Fermi liquid) associated with strict BCS theory. The normal state of, for example, a unitary gas consists of pre-formed pairs which persist below T_c in the form of non-condensed pair excitations of the condensate. This excitation branch is in addition to the usual gapped fermionic excitations. The normal state is often said to exhibit a “pseudogap” which has features in common with the exotic normal state of the high temperature superconductors. This pseudogap [4, 7] reflects the formation of quasi-bound pairs which in turn require an energy input (called Δ) in order to break the pairs and create fermionic excitations. Physically, what differs from one crossover theory to another [4, 7, 8, 9] is the nature of these non-condensed or pre-formed pairs which, respectively, appear below and above T_c . Unlike the pair fluctuations of traditional superconductors (which are associated with low dimensionality and impurity effects) these pairs are present because of a stronger-than-BCS attractive interaction. As a consequence, the pairing gap Δ persists to temperatures which can be several times T_c for the case of the unitary gases.

In this paper we address the temperature dependence of the spectral function particularly in the normal state. The density of states (DOS), which can be obtained from the spectral function, will also be presented. We compare with experiments in the context of RF spectra of both unpolarized and polarized Fermi gases. Quantum Monte Carlo simulations [10, 11] provide useful information such as the superfluid transition temperature T_c , entropy, condensate fraction, etc. and recently reveal evidence of non-condensed pairs [12] along with a pseudogap [13] in the normal phase. Our focus is on two different finite-temperature BCS-BEC crossover theories and we present a detailed comparison of the results

obtained from the two theories as well as an assessment of other BCS-BEC crossover theories.

1. Analysis of Different Crossover Theories

A fair amount of controversy [4, 14, 15, 16] has surfaced in the literature regarding the three alternative analytic pairing fluctuation schemes. In this paper we address some of these issues and clarify misleading claims. At this early stage of understanding we do not believe it is suitable to invoke (possibly fortuitous) fits to particular experimental or Monte-Carlo derived numbers to establish which of these theories is “best”. Rather in line with the goal of this paper, one has to look at the differences at a more general level. One has, furthermore, to subject these theories to careful consistency tests.

Each of the three many body approaches is associated with a different ground state. Thus far, only one of these can be written down analytically. In this context we note that one can trace the historical origin of the BCS-BEC literature to the observation that the simplest BCS-like wavefunction

$$\Psi_0 = \Pi_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger)|0\rangle, \quad (1)$$

is much more general than originally presumed [17, 18, 19]. To implement this generalization, all that is required is that one solve for the two variational parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ in concert with a self consistent condition on the fermionic chemical potential μ . As the attraction is increased, μ becomes different from the Fermi energy E_F , and in particular, in the BEC regime, μ is negative. This ground state is often called the “BCS-Leggett” state and the two variational parameters $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ can be converted to two more physically accessible parameters associated with the zero temperature gap (or equivalently order parameter) and μ .

The three theories currently of interest can be related to a t-matrix scheme. Within a given t-matrix scheme one treats the fermionic self energy and the pair-propagator using a coupled equation scheme, but drops the contributions from higher order Green’s functions. This t-matrix is called $t_{pg}(Q)$, where $Q = (i\Omega_l, \mathbf{q})$ is a four-vector and Ω_l denotes the boson Matsubara frequency; it characterizes the non-condensed pairs which are described physically and formally in different ways in the different theories. Here the subscript *pg* is associated with the pseudogap (*pg*) whose presence is dependent on the non-condensed or pre-formed pairs. Quite generally we can write the t-matrix in a ladder-diagram series as

$$t_{pg}(Q) = \frac{U}{1 + U\chi(Q)},$$

where $\chi(Q)$ is the pair susceptibility and U denotes the attractive coupling constant.

The Nozières-Schmitt-Rink (NSR) theory [19] is associated with a pair susceptibility $\chi(Q)$ which is a product of two bare Green’s functions. The fluctuation exchange or FLEX approach is associated with two dressed Green’s functions and has been discussed by Haussmann [20, 21], Zwerger and their collaborators in the context of the cold gases, and even earlier

in the context of the cuprates [22, 23, 24]. It is also called the Luttinger-Ward formalism [16], or Galitskii-Feynman theory [25]. Finally, it is well known [26, 27, 28] that BCS theory (and now its BCS-BEC generalization) is associated with one bare and one dressed Green’s function in the pair susceptibility.

These differences would seem to be rather innocuous and technical but they have led to significant qualitative differences and concurrently strong claims by various proponents. We stress that while there are several variants, as we discuss below, the version of the NSR scheme which seems to us most free of concerns is that discussed in References [7] which introduced a more physical treatment of the number equation. This revision of strict NSR theory was, in part, an answer to J. Serene [29] who raised a question about a central approximation in the theory in which the number equation ($n = 2 \sum_K G(K)$, where $G(K)$ is the single particle Green’s function) is approximated by $n = -\frac{\partial \Omega_{th}}{\partial \mu}$, where the thermodynamical potential Ω_{th} is approximated by a ladder-diagram series. It was shown that this amounts to taking the leading order in a Dyson series for $G(K)$.

The present paper concentrates on the normal state behavior, although all three classes of theories have been extended below T_c . What is essential about these extensions is that the non-condensed pair excitations associated with t_{pg} are gapless, as in boson theories. Indeed, it is in these $T \leq T_c$ extensions that a number of concerns have been raised. In particular, in the leading order extended NSR theory (or so called “Bogoliubov level” approach), [9, 30, 31], the gap equation (which is assumed to take the usual BCS form, rather than derived, for example, variationally) does not contain explicit pairing fluctuation contributions; these enter indirectly only via the fermion chemical potential μ . At this level, the number equation is the only way in which explicit pairing fluctuations are incorporated. At the so called “Popov level” calculation, the gap equation is presumed to contain pair fluctuations [32] but there is some complexity in ensuring the concomitant gaplessness of the pair excitations. Similar issues arise with the FLEX or Luttinger-Ward approach in which ([16] and references therein) gapless sound modes must be imposed somewhat artificially.

While the order of the transition at T_c is second order in the BCS-Leggett scheme it is first order [8, 9] in NSR based approaches (as well as for the fully renormalized pair susceptibility scheme. This leads to unwanted features in the density profiles [30] and T dependent superfluid density [33], $\rho_s(T)$. Despite these unphysical aspects, the NSR-based scheme captures the physics of Bogoliubov theory of weakly interacting bosons [30] and should, in principle, be the quantitatively better low T state, particularly in the BEC limit. Nevertheless some issues have been identified [34] which suggest the breakdown of true quasi-particles associated with Bogoliubov-like theories for paired fermions. This, in turn, derives from the self consistent treatment of coupling between the non-condensed pairs and the sound modes. Further analysis will be required to establish if this is compatible with experimental or theoretical constraints.

A very early concern about the so-called “GG” or FLEX

approach was raised in a paper by Kadanoff and Martin [26] in 1961: “The similarity [to a Bethe-Salpeter equation] has led several people to surmise that the symmetrical equation [involving fully dressed G ’s everywhere] solved in the same approximation would be more accurate. This surmise is not correct. The Green’s functions resulting from that equation can be rejected in favor of those used by BCS by means of a variational principle.” Importantly this approach does not have a true pseudogap. Despite claims by the Zwerger group [16] that theirs is a more fully “consistent” theory, and in this context appealing to Ref. [35], the authors of Ref. [35] instead say: “We thus conclude that ... approaches such as FLEX are unreliable in the absence of a Migdal theorem and that there is indeed a pseudogap.” Similar observations have appeared elsewhere in the literature [22, 24, 35, 36]. As noted in Ref. [36] “vertex corrections to the self energy, which are discarded in the previous studies [of FLEX] are crucially important for the pseudogap”. Additional concerns have been noted recently [25] that in the FLEX (or GG t-matrix) theory the propagator G does not display quasiparticle poles associated with the gap. “This is because the Dyson equation, $G(k) = 1/(z - \mathbf{k}^2/2m - \Sigma(k))$, excludes identical poles of G and Σ while the linear relation demands them”.

In recent work below T_c [9, 31, 37] a non-variational gap equation was used to derive an additional term in the number equation related to $\partial\Omega_{th}/\partial\Delta_{sc} \neq 0$. Here Δ_{sc} is the order parameter and, here, again, Ω_{th} is the thermodynamical potential. This extra term means there is no variational free energy functional, such as required by Landau-Ginsburg theory. Of concern are arguments that by including $\partial\Omega_{th}/\partial\Delta_{sc} \neq 0$, it is possible to capture the results of Petrov et al [38] for the inter-boson scattering length. We see no physical connection between the exact four-fermion calculations and the non-variational component of the many body gap equation. It should, moreover, be stressed that all other t-matrix schemes have reported an effective pair-pair scattering length given by $a_B = 2a$ which is larger than the value $a_B = 0.6a$ obtained from a four-body problem [38]. Here a is the s -wave scattering length of fermions. Indeed, our past work [39] and that of Reference [32] have shown that one needs to go beyond the simple t-matrix theory to accommodate these four-fermion processes.

Additional concerns arise from the fact that an NSR-based scheme has difficulty [40, 41] accommodating polarization effects in the unitary regime. As stated by the co-workers in Reference [41]: “Unfortunately, in a region around the unitary limit we find that the NSR approach generally leads to a negative population imbalance at a positive chemical potential difference implying an unphysical compressibility”.

The central weakness of the BCS-Leggett approach (and its finite- T extension) appears to be the fact it focuses principally on the pairing channel and is not readily able to incorporate Hartree effects. The evident simplicity of this ground state has raised concern as well. Clearly, this is by no means the only ground state to consider but, among all alternatives, it has been the most widely applied by the cold gas community including the following notable papers [42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52]. The central

strengths of the finite- T extended BCS-Leggett approach in comparison with others are that (i) there are no spurious first order transitions and (ii) the entire range of temperatures is accessible. (iii) Moreover, polarization effects may be readily included [53, 54], (iv) as may inhomogeneities which are generally treated using Bogoliubov deGennes theory [50, 51], based on this ground state.

The above analysis leaves us with two theoretical schemes which we wish to further explore: the NSR approach (which in the normal phase follows directly from the original paper [19]) and the BCS-Leggett-based scheme, as extended away from zero temperature, and in particular above T_c . As t-matrix approaches to many body theory, these are similar in spirit, but different in implementation. It is clearest below T_c , that the two theories focus on different physics. NSR approaches view the dominant processes as the coupling of the order parameter collective modes to the non-condensed pairs and the BCS-Leggett scheme focuses on the steady state equilibrium between the gapped fermions and the non-condensed pairs. Thus NSR focuses more fully on the bosonic degrees of freedom and BCS-Leggett focuses on the fermionic degrees of freedom. Above T_c , because the NSR scheme involves only bare Green’s functions, it is simpler. Thus, it has been studied at a numerical level in a more systematic fashion. In the literature, the BCS-Leggett approach at $T \neq 0$, has been addressed numerically [25, 55, 56, 57], assessed more theoretically [22], as well as applied to different physical contexts [58, 59, 60]. In this paper we apply an approximation based on prior numerical work [55, 56] to simplify the calculations.

2. The Fermionic Spectral Function

A central way of characterizing these different BCS-BEC crossover theories is through the behavior of the fermionic spectral function, $A(\mathbf{k}, \omega)$. For the most part, here, we restrict our consideration to the normal state where $A(\mathbf{k}, \omega)$ should indicate the presence or not of a pseudogap. A momentum integrated form of the spectral function is reflected in radio frequency studies— both tomographic [61] or effectively homogeneous and trap averaged [62, 63]. One of the principal observations of this paper is that these momentum integrated probes are not, in general, sufficiently sensitive to pick up more than gross differences between the three crossover theories.

However, there are now momentum resolved RF studies [64] which probe the spectral function more directly, in a fashion similar to angle-resolved photoemission spectroscopy (ARPES) probes of condensed matter. A central aim of this paper is to show how these studies in future will be able to differentiate more clearly between the different crossover schools. Here we confine our attention to homogeneous systems, although experiments are necessarily done for the trapped case. In addition to RF spectroscopy, it was proposed [65] that the spectral function can also be measured in Raman spectroscopy.

We note that for the HTSCs, ARPES studies have been centrally important in revealing information about the supercon-

ducting as well as the pseudogap phases [66]. Indeed, the close relation between ARPES and radio frequency probes has been discussed in our recent review [67]. It was shown in Ref. [68] that the spectral function of HTSCs in the pseudogap phase appears to exhibit dispersion features similar to those in the superconducting phase. This spectral function is modeled [55, 56, 69] by a broadened BCS form with a self energy

$$\Sigma_{pg}(K) \approx \frac{\Delta_{pg}(\mathbf{k})^2}{\omega + \epsilon_{\mathbf{k}} - \mu + i\gamma} \quad (2)$$

Here $\Delta_{pg}(\mathbf{k})$ is the (*s* or *d*-wave) excitation gap of the normal phase and γ is a phenomenological damping. Frequently, one adds an additional, structureless imaginary damping term $i\Sigma_0$, as well. High temperature superconductor experiments at temperatures as high as $T \approx 1.5T_c$ have reported that in the regions of the Brillouin zone (where the pseudogap is well established), the dispersion of the fermionic excitations behaves like

$$E_{\mathbf{k}} \approx \pm \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta_{pg}(\mathbf{k})^2} \quad (3)$$

Importantly Eq. (3) has also been used in the cold gas studies [64] in the region near and above T_c and implemented phenomenologically below T_c [65]. This both demonstrates the presence of pairing and ultimately provides information about the size of the pairing gap. It has been shown that Eq. (2) is reasonably robust in the extended BCS-Leggett state above T_c , at least up to temperatures [55, 56] of the order of $\approx 1.3T_c$. By contrast this approximate self energy is not generally suitable to NSR theory [55, 56], although for $T/T_c = 1.001$ a fit to Eq. (3) has been obtained. In a similar context we note that in the FLEX approach, the spectral function and associated self energy is not of the broadened BCS form. Mathematically, this BCS-like structure in the self energy and fermionic dispersion (which is numerically obtained) comes from the facts that the effective pair chemical potential $\mu_{pair} \rightarrow 0$ at and below T_c , and that by having one bare and one dressed Green's function in $\chi(Q)$ there is a gap in the pair excitation spectrum so that the pairs are long lived; in this way γ (which scales with the inverse pair lifetime) is small. Physically, we can say that this behavior reflects the stability of low momentum pairs near T_c and below.

These differences between the three different crossover theories become less apparent for the momentum integrated RF signals. In the BCS-Leggett approach at low temperatures the dominant structure comes from pair breaking of the condensate (which would be associated with the negative root in Eq. (3)). Despite the fact that their fermionic dispersions are different, both other theories yield a very similar “positive detuning branch” in the RF spectrum [16, 70]. However, at higher temperatures, both for polarized and unpolarized gases, there is theoretical evidence of the “negative detuning branch” arising from the positive root in Eq. (3) in the BCS-Leggett based approach [67, 71]. This is absent in the two other schemes, at least within the normal state. It also appears to be difficult to see experimentally in the unpolarized

case, although it is clearly evident once even a small polarization [47, 63] is present [72].

This paper is organized as follows. Sections II and III briefly review NSR theory and BCS-Leggett theory as extended to non-zero T . Section IV addresses a comparison of the spectral function at unitarity and on the BEC side obtained from the two theories. In subsections IV B we plot a comparison of the related density of states at unitarity and in IV C we address a comparison of RF spectra in the two theories for an unpolarized Fermi gas which also addresses experimental data. Also included is a prediction of RF spectra on the BEC side of resonance. The remaining sections (Section V and Section VI) do not focus on comparisons because the issues discussed pertain to questions which only BCS-Leggett theory has been able to address. Here we propose a subtle signature of the superfluid transition in Section V which could be addressed in future and in Section VI we address the theoretical RF spectrum of polarized Fermi gases at unitarity and its comparison with experimental data. Section VII concludes this paper.

We remark that in this paper we study *s*-wave pairing in three spatial dimensions which is more relevant to ultra-cold Fermi gases while HTSCs should be modeled as *d*-wave pairing in quasi-two dimensions. However, as one will see, there are many interesting common features in these two systems.

II. NSR THEORY ABOVE T_c

The normal state treatment of NSR theory which we apply here follows directly from the original paper in Ref. [19]. Here the different variants of NSR theory as introduced by different groups [9, 15, 30, 32] are not as important. Although there is still the concern [29] that the number equation is only approximate, the numerics are simpler if we follow the original approach; comparisons with more recent work in Ref. [73] (based on the fully consistent number equation ($n = 2 \sum_K G(K)$)) seem to validate this simplification. This same more consistent number equation is used throughout the work by the Camerino group [7].

NSR theory builds on the fact that the fermion-fermion attraction introduces a correction to the thermodynamic potential: $\Delta\Omega_{th} = \Omega_{th} - \Omega_f = \sum_Q \ln[U^{-1} + \chi_0(Q)]$, where Ω_f is the thermodynamic potential of a non-interacting Fermi gas, $\chi_0(Q)$ is the NSR pair susceptibility, and $\sum_Q = T \sum_l \sum_{\mathbf{q}}$. In the normal phase,

$$\begin{aligned} \chi_0(Q) &= \sum_K G_0(K)G_0(Q-K) \\ &= \sum_{\mathbf{k}} \frac{f(\xi_{\mathbf{k}+\mathbf{q}/2}) + f(\xi_{\mathbf{k}-\mathbf{q}/2}) - 1}{i\Omega_l - (\xi_{\mathbf{k}+\mathbf{q}/2} + \xi_{\mathbf{k}-\mathbf{q}/2})}. \end{aligned} \quad (4)$$

Here $K = (i\omega_\nu, \mathbf{k})$ where ω_ν is the fermion Matsubara frequency, $\sum_K = T \sum_\nu \sum_{\mathbf{k}}$, $G_0(K) = 1/(i\omega_\nu - \xi_{\mathbf{k}})$ is the non-interacting fermion Green's function, $\xi_{\mathbf{k}} = k^2/2m - \mu$ where m and μ denote the mass and chemical potential of the fermion, and $f(x)$ is the Fermi distribution function. We set

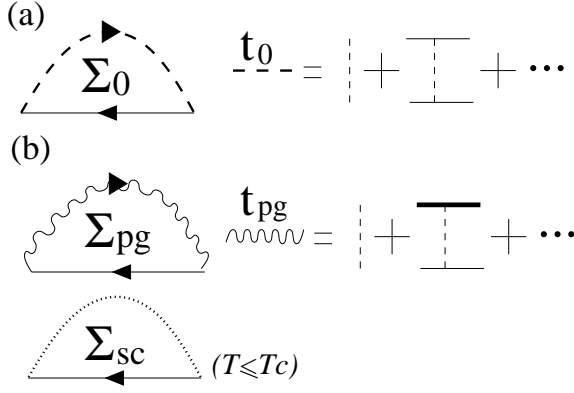


Figure 1: Fermion self-energy and ladder diagrams in (a) NSR theory and (b) $G G_0$ t-matrix theory. The thin solid line, thick solid line, thick dashed line, dotted line, wavy line, vertical thin dashed line denote G_0 , G , t_0 , $t_{sc} = -\Delta_{sc}^2 \delta(Q)/T$, t_{pg} , U .

$\hbar \equiv 1$ and $k_B \equiv 1$. NSR theory is constrained by the condition $U^{-1} + \chi_0(0) > 0$ since $U^{-1} + \chi_0(0) = 0$ signals an instability of the normal phase and the system becomes a superfluid as temperature decreases.

The fermion chemical potential is determined via the NSR number equation

$$n = -\partial \Omega_{th} / \partial \mu, \quad (5)$$

where n is the total fermion density. As noted in [19], when $\mu < 0$, $U^{-1} + \chi_0(i\Omega_l \rightarrow \Omega + i0^+, \mathbf{q}) = 0$ has solutions which correspond to bound states. Those bound states have contributions proportional to $b(\Omega_{\mathbf{q}}^{(0)})$ to the total density, where $b(x)$ is the Bose distribution function and $\Omega_{\mathbf{q}}^{(0)}$ is the energy dispersion of the bound states.

The NSR Green's function is $G(K) = [G_0(K) - \Sigma_0(K)]^{-1}$ and its retarded form is $G_R(\omega, \mathbf{k}) = G(i\omega_n \rightarrow \omega + i0^+, \mathbf{k})$. Following a t-matrix formalism, one can also consider the corrections to the fermion self-energy $\Sigma_0(K) = \sum_Q t_0(Q) G_0(Q - K)$. Figure 1 illustrates the structure of fermion self-energy in NSR theory and in the finite temperature theory associated with the BCS-Leggett ground state, which will be summarized in the next section. Here the t-matrix is given by $t_0(Q) = 1/[U^{-1} + \chi_0(Q)]$. The retarded form of the fermion self-energy has the structure $\Sigma_0(i\omega_\nu \rightarrow \omega + i0^+, \mathbf{k}) = \Sigma'_0(\omega, \mathbf{k}) + i\Sigma''_0(\omega, \mathbf{k})$, where Σ'_0 and Σ''_0 correspond to the real and imaginary part of the self-energy. We separate the contribution of the bound states from the rest (called the continuum contribution). The continuum contribution is

$$\begin{aligned} \Sigma'_{0c}(\mathbf{k}, \omega) &= \sum_{\mathbf{q}} \left\{ f(\xi_{\mathbf{q}}) \text{Re}[t_{0R}(\mathbf{q} + \mathbf{k}, \omega + \xi_{\mathbf{q}})] + \right. \\ &\quad \left. \mathcal{P} \int_{-\infty}^{\infty} \frac{d\Omega}{\pi} \frac{b(\Omega)}{\Omega - \omega - \xi_{\mathbf{q}}} \text{Im}[t_{0R}(\mathbf{q} + \mathbf{k}, \Omega)] \right\}, \\ \Sigma''_{0c}(\mathbf{k}, \omega) &= \sum_{\mathbf{q}} [b(\omega + \xi_{\mathbf{q}}) + f(\xi_{\mathbf{q}})] \text{Im}[t_{0R}(\mathbf{q} + \mathbf{k}, \omega + \xi_{\mathbf{q}})]. \end{aligned} \quad (6)$$

Here $t_{0R}(\Omega, \mathbf{q}) = t_0(i\Omega_l \rightarrow \Omega + i0^+, \mathbf{q})$ and \mathcal{P} denotes the Cauchy principal integral. In the presence of bound states, $t_{0R}(\Omega, \mathbf{q})$ has poles which result in bound state contributions to the fermion self-energy

$$\begin{aligned} \Sigma'_{0b}(\mathbf{k}, \omega) &= -\mathcal{P} \sum_{\mathbf{q}} b(\Omega_{bs}) \frac{1}{\frac{\partial \text{Re}[t_{0R}^{-1}]}{\partial \Omega} \Big|_{\Omega_{bs}}} \left[\frac{1}{\Omega_{bs} - \omega - \xi_{\mathbf{q}-\mathbf{k}}} \right] \\ \Sigma''_{0b}(\mathbf{k}, \omega) &= -\sum_{\mathbf{q}} \pi b(\Omega_{bs}) \frac{1}{\frac{\partial \text{Re}[t_{0R}^{-1}]}{\partial \Omega} \Big|_{\Omega_{bs}}} \delta(\Omega_{bs} - \omega - \xi_{\mathbf{q}-\mathbf{k}}). \end{aligned} \quad (7)$$

Here $\Omega_{bs} = \Omega_{bs}(\mathbf{q})$ denotes the location of the pole in t_{0R} .

III. BCS-LEGGETT THEORY: BROKEN SYMMETRY PHASE

We first review BCS-Leggett theory as it has been applied in the broken symmetry phase. The first three equations below represent a t-matrix approach to the derivation of the *standard* BCS gap equation. In this way we set up a machinery which is readily generalized to include BCS-BEC crossover theory. BCS theory can be viewed as incorporating *virtual* non-condensed pairs. Because they are in equilibrium with the condensate, the non-condensed pairs must have a vanishing “pair chemical potential”, $\mu_{pair} = 0$. Stated alternatively they must be gapless. The t-matrix can be derived from the ladder diagrams in the particle-particle channel (see Fig. 1):

$$t_{pg}(Q) \equiv \frac{U}{1 + U \sum_K G(K) G_0(-K + Q)}, \quad (8)$$

with $t_{pg}(Q = 0) \rightarrow \infty$, which is equivalent to $\mu_{pair} = 0$, for $T \leq T_c$. Here G , and G_0 represent dressed and bare Green's functions, respectively. To be consistent with the BCS ground state of Eq. (1), the self energy is

$$\begin{aligned} \Sigma_{sc}(K) &= \sum_Q t_{sc}(Q) G_0(-K + Q) \\ &= -\sum_Q \frac{\Delta_{sc}^2}{T} \delta(Q) G_0(-K + Q) \\ &= -\Delta_{sc}^2 G_0(-K). \end{aligned} \quad (9)$$

$\Delta_{sc}(T)$ is the order parameter while $\Delta(T)$ is the pairing gap. From this one can write down the full Green's function, $G(K) = [G_0^{-1}(K) - \Sigma_{sc}(K)]^{-1}$. Finally, Eq. (8) with $\mu_{pair} = 0$ gives the BCS gap equation below T_c :

$$1 = -U \sum_{\mathbf{k}} \frac{1 - 2f(E_k^{sc})}{2E_k^{sc}} \quad (10)$$

with $E_k^{sc} \equiv \sqrt{(\epsilon_k - \mu)^2 + \Delta_{sc}^2}$. We have, thus, used Eq. (8) to derive the standard BCS gap equation within a t-matrix language and the result appears in Eq. (10). Eq. (8) above can be viewed as representing an extended version of the Thouless criterion of strict BCS which applies for all $T \leq T_c$.

This derivation leads us to reaffirm the well known result [26, 27, 28] that BCS theory is associated with one bare and one dressed Green's function in the pair susceptibility.

Next, to address BCS-BEC crossover, we feed back the con-

tribution of the non-condensed pairs which are no longer virtual as they are in strict BCS theory, above. Eq. (8) is taken as a starting point. Equation (9) is revised to accommodate this feedback. Throughout, K, Q denote four-vectors.

$$\Sigma(K) = \sum_Q t(Q)G_0(-K+Q) = \sum_Q [t_{sc}(Q) + t_{pg}(Q)]G_0(-K+Q) = \Sigma_{sc}(K) + \Sigma_{pg}(K) \quad (11)$$

$$\text{Numerically, } \Sigma_{pg}(K) \approx \frac{\Delta_{pg}^2}{i\omega_\nu + \epsilon_{\mathbf{k}} - \mu + i\gamma} + i\Sigma_0; \text{ analytically, } \Sigma_{sc}(K) = \frac{\Delta_{sc}^2}{i\omega_\nu + \epsilon_{\mathbf{k}} - \mu}. \quad (12)$$

$$\gamma, \Sigma_0 \text{ small: } \Sigma(K) \approx -(\Delta_{sc}^2 + \Delta_{pg}^2)G_0(-K) \equiv -\Delta^2 G_0(-K) \Rightarrow \Delta_{pg}^2 \equiv -\sum_Q t_{pg}(Q) \quad (13)$$

$$t_{pg}(Q=0) = \infty \Rightarrow 1 = -U \sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}}, \quad E_{\mathbf{k}} \equiv \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta^2}, \quad (14)$$

Note that Eqs. (9) and (11) introduce the self energy which is incorporated into the fully dressed Green's function $G(K)$, appearing in t_{pg} . Also note the number equation $n = 2 \sum_K G(K)$ is to be solved consistently:

$$n = 2 \sum_K G(K) = \sum_{\mathbf{k}} \left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} + 2 \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} f(E_{\mathbf{k}}) \right] \quad (15)$$

where $\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$.

This leads to a closed set of equations for the pairing gap $\Delta(T)$, and the pseudogap $\Delta_{pg}(T)$ (which can be derived from Eq. (13)). The BCS-Leggett approach with the dispersion shown in Eq. (14) thus provides a microscopic derivation for the pseudogap model implemented in Ref. [65]. To evaluate $\Delta_{pg}(T)$ numerically, we assume the main contribution to $t_{pg}(Q)$ is from non-condensed pairs with small Q , which is reasonable if temperature is not too high [55, 56]. The inverse of t_{pg} after analytical continuation is approximated as $t_{pg}(\omega, \mathbf{q}) \approx [Z(\Omega - \Omega_{\mathbf{q}}^0 + \mu_{pair}) + i\Gamma_Q]^{-1}$, where $Z = (\partial\chi/\partial\Omega)|_{\Omega=0, q=0}$, $\Omega_{\mathbf{q}}^0 = q^2/(2M_b)$ with the effective pair mass $M_b^{-1} = (1/3Z)(\partial^2\chi/\partial q^2)|_{\Omega=0, q=0}$ which takes account of the effect of pair-pair interactions. Near T_c , $\Gamma_Q \rightarrow 0$ faster than q^2 as $q \rightarrow 0$. Following this approximation, $\Delta_{pg}(T)$ essentially vanishes in the ground state where $\Delta = \Delta_{sc}$.

The entire derivation contains one simplifying (but not fundamental) approximation. Detailed numerical calculations [55, 56] show that Σ_{pg} can be written as in Eqs. (2), which is the same as that in Eq. (12), with the observation that as T_c is approached from above, γ and Σ_0 which appears in Eq. (12) become small. To zeroth order, then, we drop γ and Σ_0 (as in Eq. (13)), and thereby can more readily solve the gap equations. To first order we include this lifetime effect as

in Eq. (12) in addressing spectral functions and other correlations.

The actual value of γ makes very little qualitative difference and the previous numerical calculations [55, 56] do not include d -wave or trap effects so that we should view γ as a phenomenological parameter. For the HTSCs, the expression for Σ_{pg} in Eq.(2) is standard in the field [69, 74, 75], and we can use specific heat jumps or angle resolved photoemission to deduce γ , as others [69] have done. For the cold gases the precise value of γ , and its T -dependence are not particularly important, as long as it is non-zero at finite T . In this paper we will deduce reasonable values for $\gamma(T)$ and Σ_0 from tomographic RF experiments.

A. Extension Above T_c

We can expand $t_{pg}(Q)$ at small Q , and in the normal state to find

$$t_{pg}^{-1}(0) \equiv Z\mu_{pair} = U^{-1} + \chi(0) \quad (16)$$

where the residue Z and pair dispersion (not shown) Ω_q , are then determined [76]. This is associated with the normal state gap equation

$$U^{-1} + \sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} = Z\mu_{pair}, \quad (17)$$

Similarly, above T_c , the pseudogap contribution to $\Delta^2(T) = \Delta_{sc}^2(T) + \Delta_{pg}^2(T)$ is given by

$$\Delta_{pg}^2 = \frac{1}{Z} \sum_{\mathbf{q}} b(\Omega_{\mathbf{q}} - \mu_{pair}). \quad (18)$$

The number equation remains unchanged. In summary, when the temperature is above T_c , the order parameter is zero, and $\Delta = \Delta_{pg}$. Since there is no condensate, μ_{pair} is nonzero, and the gap equation is modified. From these equations, one can determine μ , Δ and μ_{pair} .

B. Incorrect Criticism from the Drummond Group

The Drummond group [15] has made a number of incorrect claims about our past work which we address here. The authors claim to have numerically studied the behavior associated with the three possible pair susceptibilities. We note that there is no elemental numerical data in their paper, nor do they present details beyond their use of an “adaptive step Fourier transform” algorithm. This should be compared with work by the Tremblay group [22, 35, 77] and others [36, 57]. It is hoped that in future they will present plots of the t-matrix and self energy to the community, to the same degree that we have shared the output of our numerical schemes in References [55] and [56]. Important will be their counterparts to Figs. 8a and 9 (lower inset) in Ref. [55], which show how reliable the form in Eq. (12) is for the full GG_0 self energy. More specifically: they have argued that the “decomposition into pg and sc contributions [see Eq. (11) above], omits important features of the full theory”. This claim is incorrect and is based on their Fig. 1 of Ref. [15] which can be seen to be unrelated to the pg and sc decomposition, since their analysis of our so-called “pseudogap theory” is confined to the normal phase. *The decomposition only applies below T_c .* Moreover, we refute the argument that the decomposition into sc and pg terms shown in Eq. (11) above is unphysical. This decomposition is associated with the fact that there are necessarily both condensed and non-condensed pairs in the Fermi gases at unitarity. This break-up is standard in studies of Bose gases. The details of how to describe the pg contribution, but not its necessary presence in a decomposed fashion, are what varies from theory to theory.

Importantly, the “discrepancies” associated with thermodynamical plots based on our approach should be attributed to the absence of a Hartree term, not to any deeper physics. The reader can see that if the usual β parameter is changed from -0.41 to around -0.6 the BCS-Leggett curve will be aligned with the others.

IV. COMPARISONS OF THE SPECTRAL FUNCTION

The fermionic spectral function is given by $A(\omega, \mathbf{k}) = -2\text{Im}[G_R(\omega, \mathbf{k})]$, where G_R is the retarded Green’s function. In this section we want to explore its behavior both as a function of wavevector \mathbf{k} and of frequency ω . Of particular interest is the question of whether there is a pseudogap in the spectral function. There are different criteria for arriving at an answer. Importantly, depending of this choice the answer will be different for NSR theory (and also, it appears for the FLEX theory of Ref. [16]). The following definitions come from different measurements of HTSCs which are not internally con-

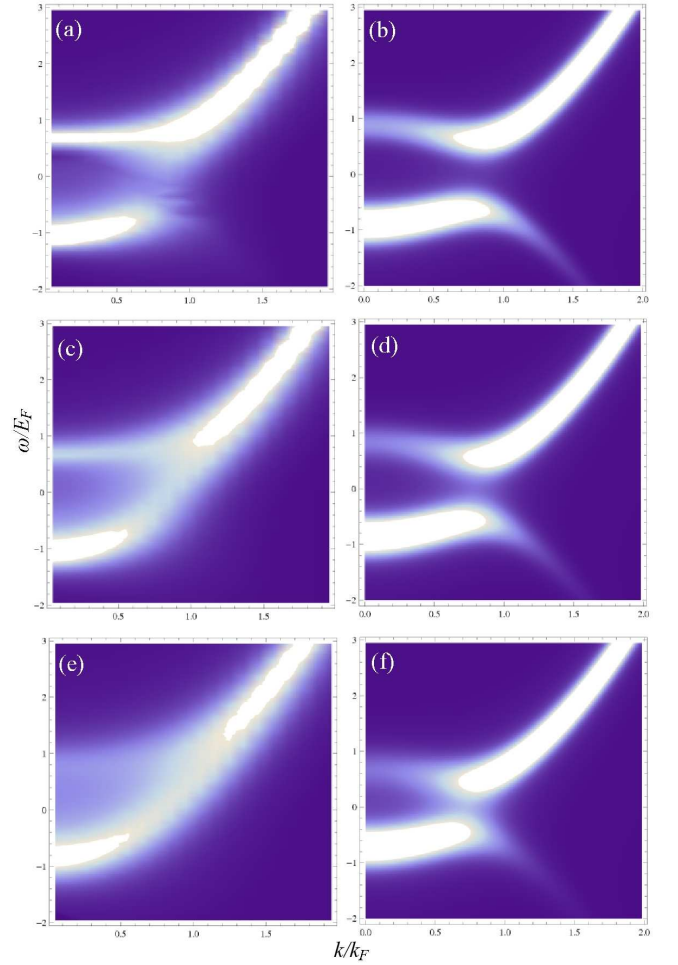


Figure 2: (Color online) Spectral function obtained from NSR theory (left column) and from the extended BCS-Leggett theory (right column) at unitarity. Temperatures (T/T_F) from top to bottom are: (a) and (b) 0.24, (c) and (d) 0.34, (e) and (f) 0.55. The ranges of k/k_F and ω/E_F are $(0, 2)$ and $(-2, 3)$, respectively.

tradictory. Following Ref. [78] and references therein, we examine two criteria for the pseudogap in HTSCs.

1. One can define the existence of a pseudogap as associated with the observation that $A(\mathbf{k}, \omega)$ as a function of ω at $k = k_F$ exhibits a two-peak structure in the normal state. This definition is particularly useful for spectroscopies such as ARPES which can probe the spectral function near the Fermi surface.
2. Alternatively, the existence of a pseudogap can be identified when the density of states (DOS) (which represents an integral over \mathbf{k} of the spectral function) is depleted near the Fermi energy. This definition appeals to tunneling experiments where the DOS can be measured.

In addressing these criteria it is useful to refer to the spectral function of the BCS-Leggett ground state given by $A_{BCS}(\omega, \mathbf{k}) = u_k^2 \delta(\omega - E_k) + v_k^2 \delta(\omega + E_k)$, where $u_k^2, v_k^2 =$

$(1/2)[1 \pm (\xi_k/E_k)]$. As a function of frequency, there are two branches: the upper branch located at $\omega = E_k$ has weight u_k^2 and the lower branch located at $\omega = -E_k$ has weight v_k^2 . Since $E_k \geq \Delta$, the spectral function is gapped at all \mathbf{k} . One recognizes two features in A_{BCS} . First, there is particle-hole mixing which results in the two branches. Second, there is an upwardly dispersing and a downwardly dispersing symmetric contribution to the spectral function arising from the \pm signs in Eq. (3). This is symmetric about the non-interacting Fermi energy. At finite temperatures, as one will see, both NSR theory and the extended-BCS-Leggett theory show particle-hole mixing in the sense that there are two branches in the spectra. In contrast, the fermionic dispersion in NSR theory does not lead to two symmetric upwardly and downwardly dispersing branches. The behavior of the finite T spectral function associated with BCS-Leggett theory, given in Eq. (2) is, however, rather similar to its superfluid analogue.

It is unlikely that Eq. (2) will be appropriate at sufficiently high temperatures. Indeed, one can see from Figure 3 in Reference [56] and the surrounding discussion that numerical calculations show this approximation is appropriate up to some temperatures of the order of $T/T_c \approx 1.3$ for a system near unitarity and in the absence of a trap. In a fully consistent numerical calculation one expects that as T is raised the pseudogap will decrease so that the pair susceptibility of the extended BCS-Leggett theory should eventually evolve from GG_0 to G_0G_0 . In this way the fully numerical NSR scheme should be very reasonable at sufficiently high T , where the pseudogap begins to break down. Physically we can argue that the BCS-Leggett scheme is better suited to treating pairs which have pre-dominantly low momentum, and thus, it should apply closer to condensation. For the purposes of comparison, in this section we apply Eq. (2) up to somewhat higher temperatures than appears strictly feasible.

A very important physical distinction emerges between the different models for the pair susceptibility which is then reflected in the fermionic self energy and ultimately in the spectral function. Because a dressed Green's function appears in BCS-Leggett theory, the t-matrix $t(Q)$ at small q has a notably different behavior, particularly at low ω as compared with the NSR case. This is seen most clearly by comparing Figure 2 and Figure 9 in Ref.[55]. This difference can be seen as a gap in the GG_0 t-matrix which serves to stabilize the pair excitations. In the normal state the pairs live longer when a pseudogap is present because of this feedback. As a result the behavior of the fermionic self energy is different, leading to a reasonable fit to Eq. (2) in GG_0 theory as shown by the lower inset in Figure 9 of Reference [55], as compared with the poorer fit to Eq. (2) found in NSR theory and shown in Figure 8a from Ref. [55]. We will reach qualitatively similar conclusions in the next section of the paper. We summarize by noting that the extended BCS-Leggett theory focuses on low q pairs which dominate near condensation. NSR theory treats pairing without singling out low q only. Each of these theories should be appropriate in different temperature regimes of the normal state. Concomitantly, because of the enhanced stability of the pairs, the broadening of the spectral peaks will be considerably smaller in BCS-Leggett theory as compared

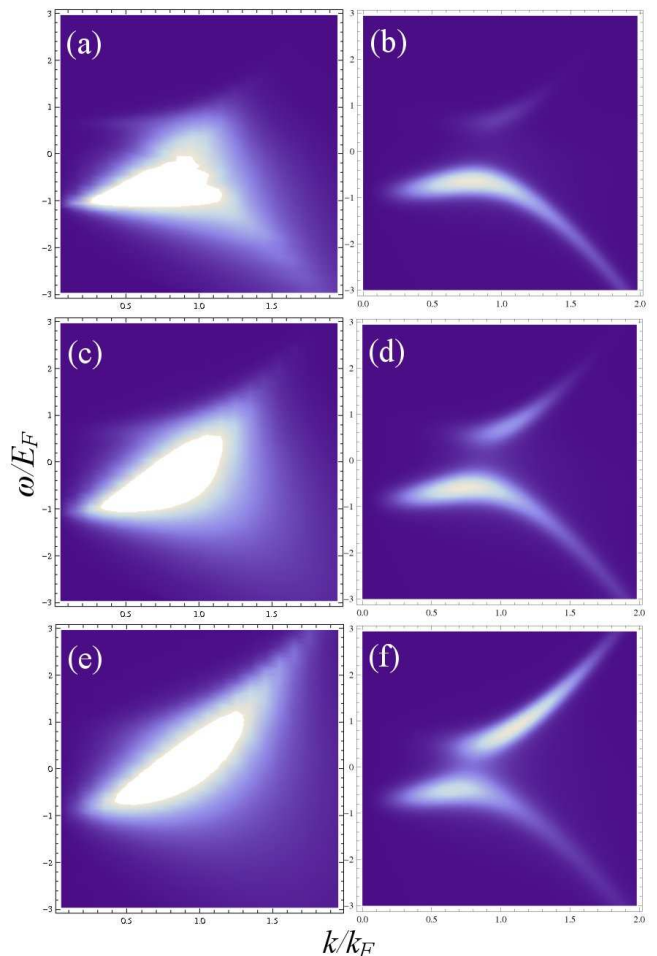


Figure 3: (Color online) The plot of the function $k^2 f(\omega) A(\mathbf{k}, \omega) / 2\pi^2$ calculated from NSR theory (left column) and from the extended BCS-Leggett theory (right column) at $1/k_F a = 0$. Temperatures (T/T_F) from top to bottom are: (a) and (b) 0.24, (c) and (d) 0.34, (e) and (f) 0.55. The ranges of k/k_F and ω/E_F are (0, 2) and $(-3, 3)$, respectively.

with NSR theory.

To make a connection with experiments on ultra-cold Fermi gases, we regularize the attractive coupling constant via $U^{-1} = m/(4\pi a) - \sum_{\mathbf{k}} (m/k^2)$. We choose as our units the Fermi energy E_F , or, as appropriate the Fermi temperature T_F , or Fermi momentum k_F of a non-interacting Fermi gas with the same particle density. The unitary point where a diverges is of particular interest because two-body bound states emerge. Since many-body effects renormalize the coupling constant, the fermion chemical potential remains positive at unitarity in both NSR theory and the BCS-Leggett theory. This implies that bound states in a many-body sense have not fully emerged. In our numerics, we choose $\gamma(T)$ to be very roughly consistent with RF experiments. For the unpolarized case we set $\gamma/E_F = 0.12(T/T_c)$ at unitarity and included a small background imaginary term $\Sigma_0/E_F = 0.05$.

A. Comparison of Spectral functions via Contour plots

Figure 2 present a plot of the spectral function at unitarity ($1/k_F a = 0$) obtained from NSR theory (left column) and from the BCS-Leggett t-matrix theory (right column) at selected temperatures. In the BCS-Leggett case we use the approximation that the self energy associated with non-condensed pairs is of a broadened BCS form (in Eq. (2)). The transition temperatures $T_c/T_F = 0.238$ and $T_c/T_F = 0.26$ are obtained for the NSR and BCS-Leggett cases respectively. Both theories yield higher T_c values than found [10] in quantum Monte Carlo simulations, where $T_c/T_F \approx 0.15$ at unitarity. The T_c curves in BCS-BEC crossover of NSR and the extended BCS-Leggett theories are shown in Ref. [14].

In Fig. 2 the comparisons are made at three different temperatures. The horizontal and vertical axes on each panel correspond to wave number and frequency and what is plotted in the contour plots is the fermionic spectral function for a three-dimensional homogeneous gas. The white areas correspond to peaks in the spectral function and they map out a dispersion for the fermionic excitations. With the possible exception of the highest T NSR case (lower left figure) the spectral functions in all cases shown in Fig. 2 are gapped at small k/k_F , which indicates the existence of particle-hole mixing. The lower branch of the spectral function from the BCS-Leggett t-matrix theory clearly shows a downward bending for $k > k_F$ which is associated with a broadened BCS-like behavior. The spectral function of a phenomenological pseudogap model presented in Ref. [65], which *can be derived microscopically from the BCS-Leggett approach*, exhibits similar contour plots as ours from the extended BCS-Leggett theory. By contrast, in NSR theory the lower branch corresponds to very broad and very small peaks when $k > k_F$ which are barely observable. We see no clear evidence of a downward dispersing branch even at the lowest temperature above T_c .

As a function of temperature, in the NSR case, the physics suggests a smooth evolution with increasing T towards a single branch, upwards dispersing—almost Fermi liquid dispersion. It seems likely that as T is raised and the pairing gap becomes less important the pair susceptibility of the BCS-Leggett state should cross from GG_0 to G_0G_0 so that the two schemes merge. This means that our previous simplification of the fermionic self energy Σ (as a broadened BCS form, see Eq. (12)) is no longer suitable in this high T regime. There are not really two different types of pseudogap, but rather the extended BCS-Leggett theory represents pairs which are close to condensation— and thus predominantly low momentum pairs. [This is built into the approximation Eq. (12), which was used to model the pseudogap self energy.] By contrast the NSR case considers pairs with a broad range of momenta.

One can see that the vanishing of the pseudogap as temperature increases is different in the two theories. In the extended BCS-Leggett theory, the two branches approach each other and the gap closes while in NSR theory, the spectral function fills in the gapped regime and its overall shape evolves toward a single parabola. We note that our spectral function from NSR theory at unitarity looks identical to the results in Ref. [73], even though the latter was computed with a

more self consistent number equation. This implies that the difference between the two number equations (Eq. (5) and $n = 2 \sum_K G(K)$) has no qualitative impact. Interestingly, the spectral function at the highest T from NSR theory resembles that presented in Ref. [16] for the near- T_c normal phase of GG t-matrix theory.

It should be noted that this spectral function is not the quantity directly measured in momentum resolved RF studies [64]. Rather what is measured there is the function $k^2 f(\omega) A(\mathbf{k}, \omega) / 2\pi^2$ which is plotted in Figure 3. This convolution preserves the large momentum part of the lower branch of the spectral function and suppresses the remainder. The downward bending behavior is clearly observed in the extended BCS-Leggett theory again (right column) for all three temperatures. In contrast, only the lowest temperature plot of NSR theory ($T/T_F = 0.24$, slightly above T_c) shows a weak downward bending at large momentum. This downward dispersion, however, cannot be observed at higher temperatures (left column). In the actual momentum-resolved RF experiments of trapped Fermi gases [64] trap averages enter so that the actual curves are substantially broader [71]. A clear signature of downward dispersion in experimental data will help determine whether the pseudogap phase with noncondensed pairs behaves in a way which is similar to the HTSCs, where this feature has been reported [68]. It should be noted that it is this signature which has been used in Ref. [64] to arrive at an indication of the presence of pairing.

The issue of what constitutes the proper definition of a pseudogap is an important one and we turn next to the first definition we introduced above in which one requires that the spectral function $A(\omega, \mathbf{k})$ as a function of ω exhibits two peaks around $k \approx k_F$. It is clearly seen that in the BCS Leggett approach this definition is met for all three curves exhibited in Figure 2. Because it is more difficult to establish this for the NSR results plotted in Fig. 2, in Fig. 4 we address this question more directly for two different temperatures and a range of k values near k_F . It should be clear that at the lower temperature (which is slightly above T_c), a pseudogap is seen in NSR theory, although we have seen that the peak dispersion is not well described by Eq. (3). This pseudogap should not be viewed as a broadened BCS like feature. At the higher temperature shown by the bottom panel of Fig. 4 there appears to be no indication of a pseudogap according to the first definition. Only a single peak is found in the spectral function near k_F .

We next explore analogous curves in the BEC regime and thereby investigate how many-body bound states affect the distribution of weight in the spectral function. Figure 5 illustrates the spectral function on the BEC side of resonance with $1/k_F a = 1$ obtained from NSR theory (left column) and from the extended BCS-Leggett theory (right column) at selected temperatures. Here $T_c/T_F = 0.22$ for the NSR case and $T_c/T_F = 0.21$ in the BCS-Leggett scheme. There is noise at small k in the spectral function of NSR theory which is presumably a numerical artifact. In the presence of bound states (in a many-body sense), the lower branch of the spectral function of NSR theory shows a downward bending near T_c , but it can be seen that this behavior rapidly evolves to an upward

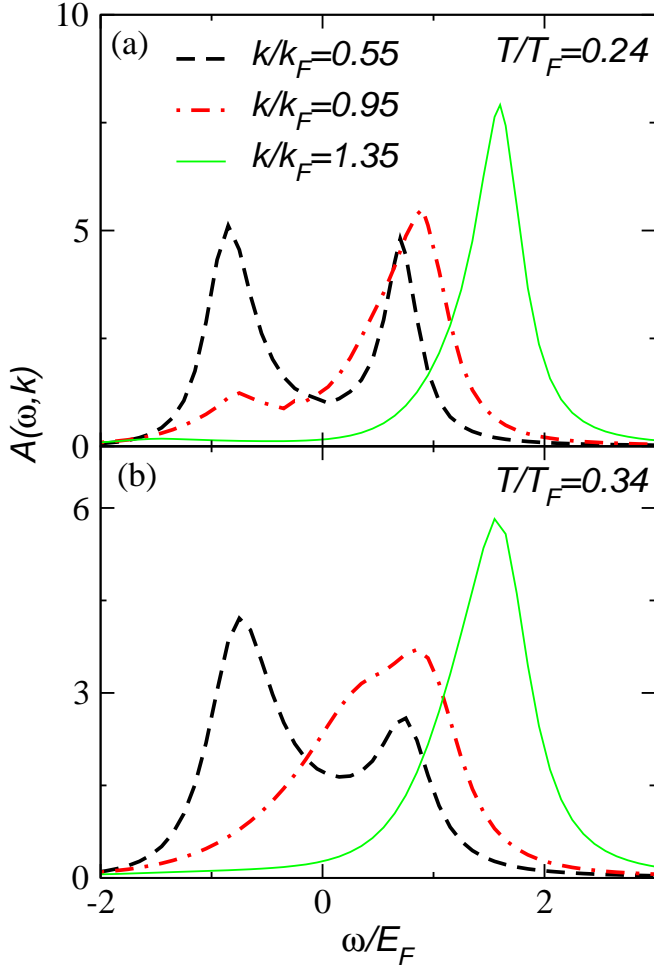


Figure 4: Behavior of the frequency dependent spectral function at unitarity in NSR case for (a) $T/T_F = 0.24$ and (b) $T/T_F = 0.34$ for various wave-vectors \mathbf{k} . This Figure suggests that the two-peak structure near k_F associated with this crossover theory barely meets the (most restrictive) definition for the presence of a pseudogap near T_c . Away from T_c , the two-peak structure near k_F is virtually not observable.

dispersion as T increases (Fig. 5(e)). In contrast, the spectral function from the extended BCS-Leggett theory exhibits the downward dispersion at all T indicated, rather similar to the behavior in the superfluid phase.

One can further see from the figure that in the extended BCS-Leggett theory the lower branch has a much weaker spectral weight compared to that of the upper branch. This derives from the same phenomenon as in the BCS-Leggett ground state, where the coefficient v_k^2 becomes negligibly small in the BEC regime. The behavior of the NSR spectral function is rather different from its counterpart in BCS-Leggett theory at all three temperatures. If one plots the spectral function at $k = k_F$ as a function of ω two peaks are present with the upper peak much sharper and narrower than the lower, as also reported in Ref. [73].

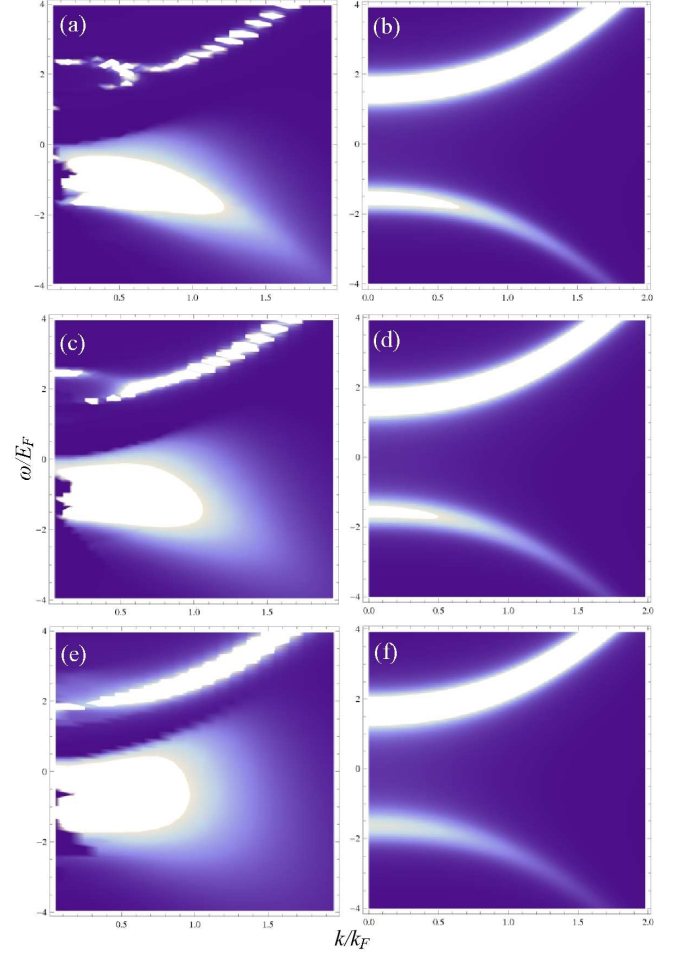


Figure 5: (Color online) Spectral function obtained from NSR theory (left column) and from the extended BCS-Leggett theory (right column) at $1/k_F a = 1$. Temperatures (T/T_F) from top to bottom are: (a) and (b) 0.25, (c) and (d) 0.34, (e) and (f) 0.55. The ranges of k/k_F and ω/E_F are $(0, 2)$ and $(-4, 4)$, respectively.

B. Comparison of Density of States

We turn now to the DOS which, when depleted around the Fermi energy, provides a second criterion for the existence of the pseudogap. The DOS is given by

$$N(\omega) = \sum_{\mathbf{k}} A(\omega, \mathbf{k}). \quad (19)$$

In the HTSCs, an above- T_c - depletion in the DOS around the Fermi energy, measured in tunneling experiments, provided a clear signature of the pseudogap ([78] and references therein). By contrast, in the ultra-cold Fermi gases the DOS has not been directly measured, although it is useful to discuss it here in an abstract sense.

Figure 6 shows the DOS from the two theories at unitarity and at selected temperatures. The DOS based on the extended BCS-Leggett theory clearly shows a pseudogap at all three selected temperatures. Similarly, the DOS from NSR theory show a clear depletion around the Fermi energy ($\omega = 0$) at

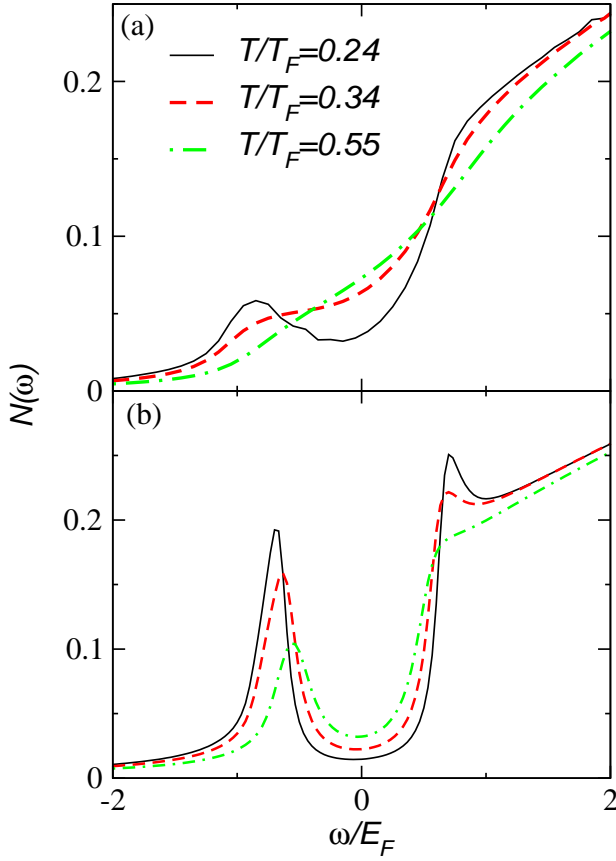


Figure 6: (Color online) DOS at unitarity from (a) NSR theory and (b) the extended BCS-Leggett theory. (Black) solid line, (red) dashed line, and (green) dot-dash line correspond to $T/T_F = 0.24$, 0.34 , and 0.55 .

$T/T_F = 0.24$. This depletion is barely visible at 0.34 . At higher temperature ($T/T_F = 0.55$), the depletion does not appear, and one sees only an asymmetric background. We note that our NSR results are similar to those in Ref. [73] although different number equations were employed. With this criterion for a pseudogap one would conclude that NSR theory does have a pseudogap — at least at $T \approx T_c$. It is somewhat unlikely that the FLEX scheme (which at T_c seems to behave similarly to the highest T NSR figures) a pseudogap would be present— via this second definition.

C. Comparison of RF Spectra of Unpolarized Fermi Gases

The RF current at detuning ν also depends on an integral involving the fermionic spectral function. The current obtained from linear response theory is given by [54]

$$I_0^{RF}(\nu) = \sum_{\mathbf{k}} \frac{|T_{\mathbf{k}}|^2}{2\pi} A(\omega, \mathbf{k}) f(\omega) \Big|_{\omega=\xi_{\mathbf{k}}-\nu}. \quad (20)$$

where, for the present purposes we ignore the complications from final-state effects [79, 80], as would be reasonable for the

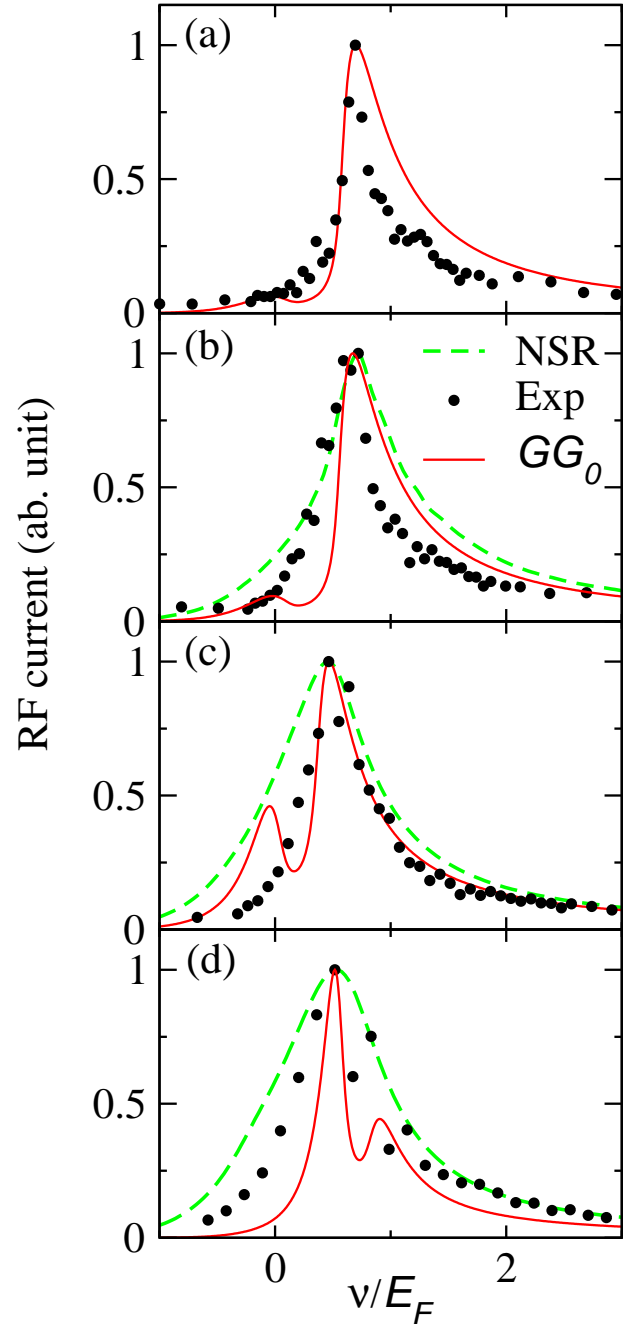


Figure 7: (Color online) RF spectrum at $1/k_F a = 0$. The (black) solid dots, (red) solid lines, and (green) dashed lines correspond to the RF currents obtained from the experimental data ([61], supplemental materials), the extended BCS-Leggett theory, and NSR theory. The values of T/T_F are (a) 0.2 , (b) 0.22 (0.24 for the curve from NSR theory), (c) 0.34 , and (d) 0.55 .

so-called “13” superfluid of ^6Li . Here $|T_{\mathbf{k}}|^2$ is a tunneling matrix element which is taken to be a constant. The data points in Figure 7 correspond to measured tomographic spectra from Ref. [61] in units of the local Fermi energy, (see the Supplemental Materials). The results from NSR theory are indicated by the dashed lines and from the extended BCS-Leggett the-

ory (GG_0) by the solid (red) lines. To compare and contrast the spectra, we normalize each curve by its maximum and align the maxima on the horizontal axis, so as to effectively include Hartree shifts. The experimental data were taken at $T/T_F = 0.2, 0.22, 0.34, 0.55$. The RF spectra from the extended BCS-Leggett theory are calculated at the same set of temperatures. The RF spectra from NSR theory, which are restricted to the normal phase correspond to the three higher temperatures: $T/T_F = 0.24, 0.34, 0.55$.

The RF spectra from the extended BCS-Leggett theory at high temperatures indicate a double-peak structure, which was addressed in Ref. [80]. This peak at negative RF detuning emerges at finite temperatures in BCS-Leggett theory as a result of thermally excited quasiparticles. With increasing T , the weight under this peak increases although the peak-to-peak separation will decrease, following the temperature dependent pairing gap, as seen in the figure. When temperature increases, the peak at negative RF detuning grows and nearly merges with the peak at positive RF detuning so that it may not be resolved experimentally.

By contrast, the RF spectra in NSR theory show a single peak which is broader than the experimental RF spectra. This is to be expected based on our analysis of the NSR spectral function in the previous section, where we saw that the symmetrical upward and downward dispersing branches of BCS theory were not present. The RF spectra presented in Ref. [16] using GG t-matrix (FLEX) theory also shows a broader (than experiment) single peak.

In view of the contrast between the BCS-Leggett curves and experiment, it is natural to ask why is there no indication of the negative detuning peak in these unpolarized experiments? One can contemplate whether this stems from the fact that (owing to large γ) the two peaks simply aren't resolved. This would yield a figure closer to that obtained from NSR-based calculations, which is associated with a rather broad peak structure. As a result it would not lead to a more satisfying fit to experiment. At this stage we have no clear answer, but it will be important to investigate, as we do below, very slightly polarized gases to gain some insight.

In Figure 8 we present the comparison on the BEC side of resonance. Here $1/k_F a = 1$ and $T/T_F = 0.34$. In this case both spectra show a double-peak structure. For convenience, we have scaled both spectra to their maxima and aligned the maxima. For the NSR case, the double-peaked feature reflects the negative fermionic chemical potential which is associated with bound states. It similarly reflects the stronger spectral weight of the upper branch in the spectral function which can also be examined in Figure 5. Our RF spectra in NSR theory are consistent with those presented in Ref. [70].

V. EXTENDED BCS-LEGGETT THEORY: SIGNATURE OF T_c IN RF SPECTRUM

We have tried in the paper to emphasize comparisons whenever possible, but there are instances where other crossover theories (besides that based on the BCS-Leggett theory) have no counterpart. In the first of these we investigate the signa-

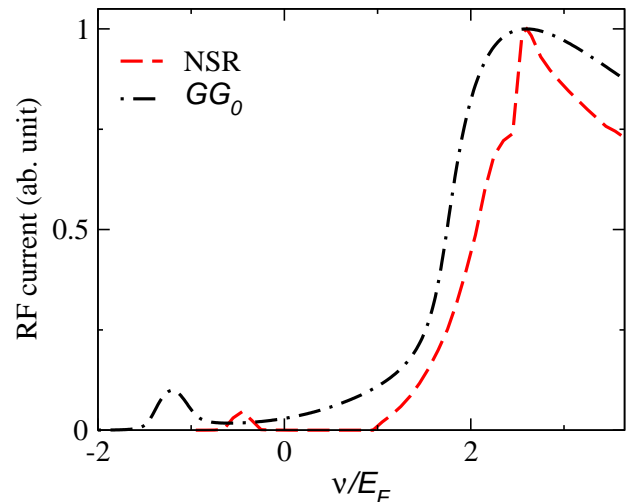


Figure 8: (Color online) RF spectrum at $1/k_F a = 1$. The (black) dot-dash line and (red) dashed line correspond to the RF currents obtained from the extended BCS-Leggett (GG_0) theory and NSR theory at $T/T_F = 0.34$.

ture of the second order transition which should be a subtle, but nevertheless thermodynamically required feature of any crossover theory. The experimental RF spectra in Ref. [61, 62] imply that the RF spectrum is more sensitive to the existence of pairing rather than to superfluidity. That it evolves smoothly across T_c is due to the presence of noncondensed pairs. The extended BCS-Leggett theory has the important advantage in that it describes a smooth transition across T_c and should be a suitable theory for investigating this question. In contrast, NSR theory and its generalization below T_c , as well as the FLEX or Luttinger-Ward approach [16] encounter unphysical discontinuities

In the following we search for signatures of T_c in the RF spectrum as obtained from BCS-Leggett theory near T_c . Here, in contrast to Ref. [67], we use constraints provided by our semi-quantitative fits to RF spectra (associated with the estimated size of $\gamma(T)$) to obtain a more direct assessment of how important these superfluid signatures should be.

Figure 9 presents a plot suggesting how one might expect to see signatures of coherence in a tomographic (but momentum integrated) RF probe, such as pioneered by the MIT group [61]. It shows the RF current versus temperature at three different detuning frequencies. The inset plots the RF characteristics indicating where the frequencies are chosen. One can see that there is a feature at T_c , as expected. This shows up more clearly in the lower figure which plots the temperature derivative. The same sort of feature has to be contained in the specific heat [81] which represents an integral over the spectral function. What does it come from, since RF is not a phase sensitive probe? The feature comes from the presence of a condensate below T_c . What is distinguishing condensed from non-condensed pairs is their self energy contribution. In the HTSCs [74] and also in the BCS-Leggett formulation the self energy from the non-condensed pairs is taken to be of a broadened BCS form in Eq. (12). By contrast, the non-condensed

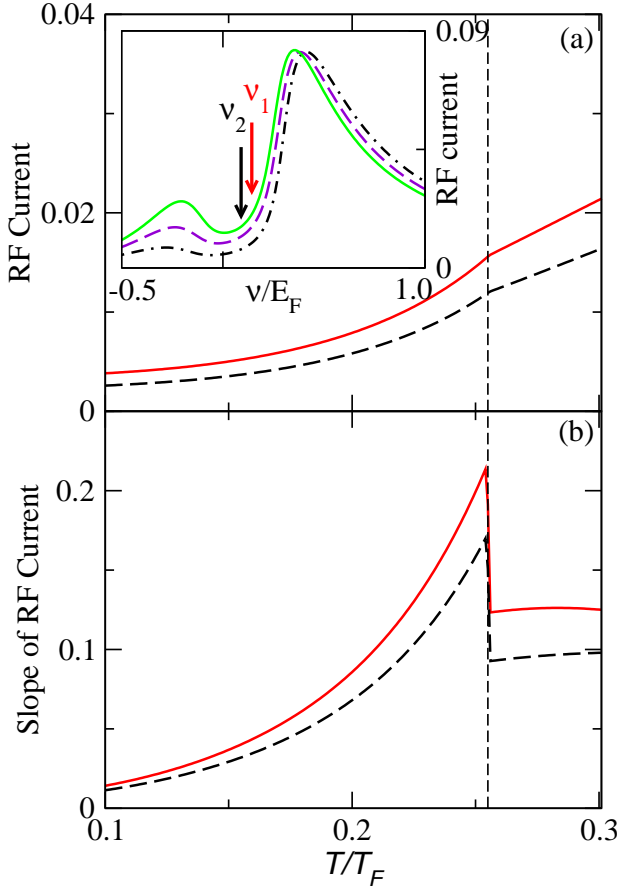


Figure 9: (Color online) (a) RF current as a function of T at $1/k_F a = 0$ for $\nu_1/E_F = 0.15$ (black dashed line) and $\nu_1/E_F = 0.1$ (red solid line) obtained from the extended BCS-Leggett theory. Inset: RF currents as a function of detuning at $T/T_F = 0.22$ (dot-dash line), 0.26 (dashed line), 0.3 (solid line). The two arrows indicate ν_1 and ν_2 . (b) The slopes of the RF currents from (a). The vertical dashed line indicates T_c .

pairs live infinitely long and so have no damping γ . These are the effects which are represented in Figure 9. In this way the figure shows that there are features at T_c which can in principle help to distinguish the ordered state from the normal pseudogap phase.

VI. EXTENDED BCS-LEGGETT THEORY: RF SPECTRUM OF POLARIZED FERMION GASES

Another strength of the BCS-Leggett approach is that it can address polarized gases at unitarity, which are not as readily treated [40, 41] in the alternative crossover theories. In Figure 10 we plot the RF spectra from the extended BCS-Leggett theory and the experimental RF spectra from Ref. [61]. Since the experimental RF spectra were obtained from RF tomography of trapped polarized Fermi gases, we follow a similar procedure to extract our RF spectra at varying, but comparable locations from a similar trap profile. Also indicated are the polarizations p . If we make fewer restrictions on the choice of ra-

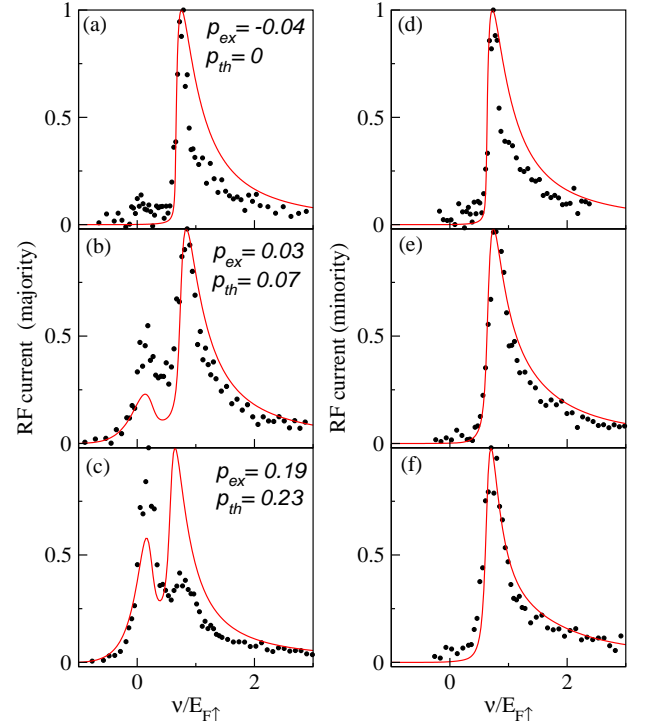


Figure 10: (Color online) RF spectra of polarized Fermi gases at unitarity. (Black) dots and (red) solid lines correspond to the experimental data from Ref. [61] and results from the extended BCS-Leggett theory. The left (right) column shows the RF spectra for the majority (minority) species. The local temperature $T/T_{F\uparrow}$ and local polarization p for the experimental data (ex) and the theoretical results (th), $(T_{ex}/T_{F\uparrow}, T_{th}/T_{F\uparrow}, p_{ex}, p_{th})$, are: $(0.05, 0.04, -0.04, 0)$ for (a) and (d); $(0.06, 0.13, 0.03, 0.07)$ for (b) and (e); $(0.06, 0.15, 0.19, 0.23)$ for (c) and (f).

dial variable, the agreement is better as is shown in Ref. [67]. To compare the results, we normalized the maxima and align the spectra, thereby introducing a fit to Hartree contributions. The left (right) column shows the RF spectra of the majority (minority). Here we set $\gamma/E_F = 0.05$ and $\Sigma_0/E_F = 0.02$.

The experimental data points from the left hand column can be compared with those in Figure 7 which are for the $p \equiv 0$ case, and it is seen that even at very small polarizations (say $p \approx 0.03$) the negative detuning peak becomes visible. Indeed, it appears here to be larger than the theoretically estimated negative detuning peak height. A possible explanation for why the double-peak structure can be resolved experimentally in polarized but not in unpolarized Fermi gases is because the existence of excess majority fermions causes a negative RF-detuning peak even at low temperatures. At these lower T the separation between the two peaks can be large in the experimental RF spectra of polarized Fermi gases. In contrast, for an unpolarized Fermi gas the negative RF-detuning peak due to thermally excited quasiparticles only becomes significant at high temperatures around T_c and above. Here the separation between the two peaks may not be as readily resolved. As expected, at low temperatures there is only a single peak in the RF spectra of the minority. We notice that at extremely high

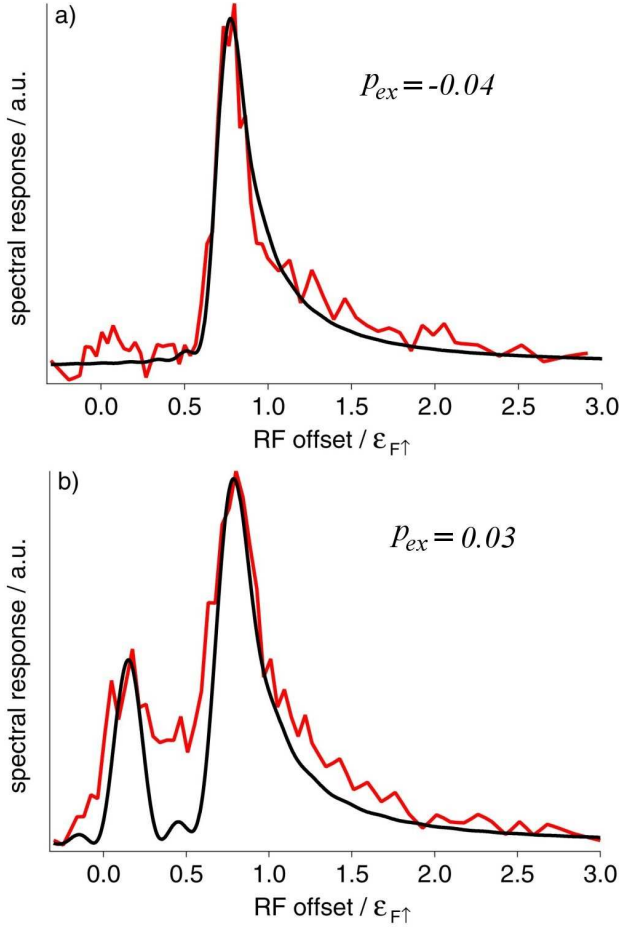


Figure 11: (Color online) Reproduction of Fig.5 in the Supplemental Materials of Ref. [72]. Red curves correspond to experimental data from Fig. 10 (a) and (b). Black curves are RF currents calculated from BCS-Leggett theory.

polarization, polaron-like behavior has been observed in RF experiments [82], whose explanation has attracted a great deal of attention in the theoretical community [83, 84]. These effects have not been incorporated in our BCS-Leggett formalism, where the normal state has been assumed to be strictly non-interacting [53].

The Ketterle group [72] has argued that it should be possible to extract the pairing gap size from RF spectroscopy in polarized gases at very low temperatures. In Fig. 11 we present a plot from their paper (Supplementary Materials) which relates to their procedure. This figure presents a fit to a generalized BCS-Leggett ground state in the presence of polarization. The red curves correspond to the actual data and the black curves are obtained from this theory. An additional resolution broadening is included in the theory and one can see that this theoretical approach appears to be in quite reasonable agreement with experiment. In this way there is some support for this simplest of ground states — at least in the polarized case.

VII. CONCLUSION

The goal of this paper is to communicate that BCS-BEC crossover theories are very exciting. They are currently being clarified and developed hand in hand with experiment. For the Fermi superfluids, unlike their Bose counterparts, we have no ready-made theory. In this paper we confine our attention to the normal phase, although we have presented a discussion of some of the controversial issues which have surface in the literature below T_c . We view the principal value of this paper is the presentation of comparisons of two different crossover theories and the identification of (mostly future) experiments which can help distinguish them. The two theories we consider are the extended BCS-Leggett theory and that of Nozieres and Schmitt-Rink. We chose not to discuss the FLEX or Luttinger-Ward scheme in any detail because it is discussed elsewhere [16], and because there are concerns that, by ignoring vertex corrections, this approach has omitted the important physics associated with the pseudogap. These concerns are longstanding [22, 24, 35, 36]. Here we have argued that the extended BCS-Leggett theory is the one theory which preserves (broadened) BCS features into the normal state over a significant range of temperatures. Even above T_c one finds that the fermionic excitations have an (albeit, smeared out) dispersion of the form $E_{\mathbf{k}} \approx \pm \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta_{pg}^2}$ in the normal state. We find that NSR theory does not have this dispersion, although it has a pseudogap by all other measures. Interestingly high T_c superconductors have been shown to have this dispersion in their normal state [68] and it is generally believed [69, 74, 75] that their fermionic self energy can be fit to a broadened (d -wave) BCS form $\Sigma_{pg}(K) \approx \Delta_{pg}(\mathbf{k})^2 / (\omega + \epsilon_{\mathbf{k}} - \mu + i\gamma)$.

In this paper we show that one can identify both physically and mathematically the difference between the two normal states of the different crossover theories. Mathematically because BCS theory involves one dressed Green's function in the pair susceptibility, it leads to a low frequency gap in the t -matrix or pair propagator (at low q). Physically this serves to stabilize low momentum pairs. This helps us to understand that the pseudogap of NSR theory does not incorporate primarily low momentum pairs, but rather pairs of all momentum and that it should be better further from condensation. Indeed, this is reinforced by our observation that at higher T , feedback effects which distinguish the two theories becomes less and less important and the BCS-Leggett pair susceptibility, GG_0 , crosses over to something closer to G_0G_0 as in NSR theory. Our simplest approximation for the self energy in Eq. (2) is no longer suitable once temperature exceeds, say $T/T_c \approx 1.5$. Indeed this is reinforced by earlier numerical observations [55, 56].

As a result, we believe that both theories are right but in different temperature regimes. Moreover, this serves to elucidate another concern about NSR theory (and FLEX theory)—that they are associated with an unphysical first order transition. Both theories change discontinuously in going from above to below T_c . In the superfluid phase the coupling which is included in all other theories is between the non-condensed pairs

and the collective modes of the condensate, even though in the normal state one couples the fermions and the non-condensed pairs. In the extended BCS-Leggett theory, (as seems reasonable, in the vicinity of T_c both above and below), the dominant coupling is, indeed, between non-condensed pairs and fermions. These (effectively, pseudogap) effects will behave smoothly across T_c . The Goldstone modes which turn on at T_c are highly damped in its vicinity, where the condensate is weak. Only at lower T should their coupling become the more important.

In summary, a central conclusion of this study of the spectral functions of the extended BCS-Leggett theory and NSR theory is that one may expect that the former is suitable near T_c due to its similarity to BCS theory while the latter better describes the normal phase at much higher T as the system approaches a Fermi liquid, and concomitantly, the pseudogap begins to disappear. In the course of this work we have found

that the theoretical RF spectra from both theories agree (only semi-quantitatively) to about the same extent with experimental data at unitarity. The BCS-Leggett approach has the advantage that it can address the RF spectrum of generally polarized Fermi gases without the problems which have been noted [41] for the NSR approach. However, momentum resolved experiments [64] may be the ultimate way of distinguishing experimentally between different theories.

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